Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	660	(544/317).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2005/10/01 09:12
L2	799	(544/320).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2005/10/01 09:12
L3	417	(544/322).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2005/10/01 09:12
L4	390	(514/252.14).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2005/10/01 09:13
L5	50	bjorn.inv. and nilsson.in.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2005/10/01 09:13

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	660	(544/317).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2005/10/01 09:12
L2	799	(544/320).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2005/10/01 09:12
L3	417	(544/322).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2005/10/01 09:12
L4	390	(514/252.14).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2005/10/01 09:13
L5	50	bjorn.inv. and nilsson.in.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2005/10/01 09:13

```
chain nodes :
    19   24   25   27   28
ring nodes :
    1   2   3   4   5   6   7   8   9   10   11   12   13   14   15   16   17   18
chain bonds :
    2-25   3-27   4-28   6-24   13-19
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   7-8   7-12   8-9   9-10   10-11   11-12   13-14   13-18   14-15
    15-16   16-17   17-18
exact/norm bonds :
    2-25   6-24   13-19
exact bonds :
    3-27   4-28   7-8   7-12   8-9   9-10   10-11   11-12   13-14   13-18   14-15   15-16   16-17   17-18
normalized bonds :
    1-2   1-6   2-3   3-4   4-5   5-6
isolated ring systems :
    containing 1 : 7 : 13 :


G1:C,O,S,N,X,Cy,[*1],[*2]

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom   10:Atom   11:Atom
    12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   18:Atom   19:CLASS   24:CLASS   25:CLASS
    27:CLASS   28:CLASS
```

Connecting via Winsock to STN

Welcome to STN International!   Enter x:x

LOGINID:sssptal611bxv

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * *   Welcome to STN International   * * * * * * * * * *

    NEWS 1   Web Page URLs for STN Seminar Schedule - N. America
    NEWS 2   "Ask CAS" for self-help around the clock
    NEWS 3   JUL 20   Powerful new interactive analysis and visualization software,
                         STN AnaVist, now available
    NEWS 4   AUG 11   STN AnaVist workshops to be held in North America
    NEWS 5   AUG 30   CA/CAplus -Increased access to 19th century research documents
    NEWS 6   AUG 30   CASREACT - Enhanced with displayable reaction conditions
    NEWS 7   SEP 09   ACD predicted properties enhanced in REGISTRY/ZREGISTRY
    NEWS 8   SEP 22   MATHDI to be removed from STN

    NEWS EXPRESS   JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT
                    MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
                    AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005

    NEWS HOURS   STN Operating Hours Plus Help Desk Availability
    NEWS INTER   General Internet Information
    NEWS LOGIN   Welcome Banner and News Items
    NEWS PHONE   Direct Dial and Telecommunication Network Access to STN
    NEWS WWW   CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
specific topic.

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   research. Use for software development or design or implementation
   of commercial gateways or other similar uses is prohibited and may
   result in loss of user privileges and other penalties.

   * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 07:40:13 ON 01 OCT 2005

=> file reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                    ENTRY   SESSION
FULL ESTIMATED COST   0.21   0.21

FILE 'REGISTRY' ENTERED AT 07:40:21 ON 01 OCT 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 29 SEP 2005   HIGHEST RN 864227-43-0
DICTIONARY FILE UPDATES: 29 SEP 2005   HIGHEST RN 864227-43-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

    Please note that search-term pricing does apply when
   conducting SmartSELECT searches.

****
*   *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005. A new display format, IDERL, is now   *
* available and contains the CA role and document type information. *
*   *
****

Structure search iteration limits have been increased. See HELP SLIMITS
for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Documents and Settings\VBalasubramania\My
Documents\STNEXP4\QUERIES\106188682.str

chain nodes :
19 24 25 27 28
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
chain bonds :
2-25 3-27 4-28 6-24 13-19
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18
14-15 15-16 16-17 17-18

exact/norm bonds :
2-25 6-24 13-19
exact bonds :
3-27 4-28 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16 16-17
17-18
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 : 7 : 13 :

G1:C,O,S,N,X,Cy,[*1],[*2]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS
24:CLASS 25:CLASS 27:CLASS 28:CLASS

L1   STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1   STR
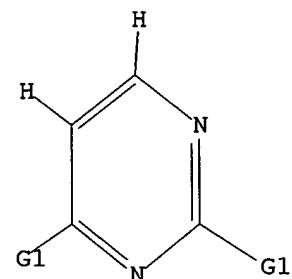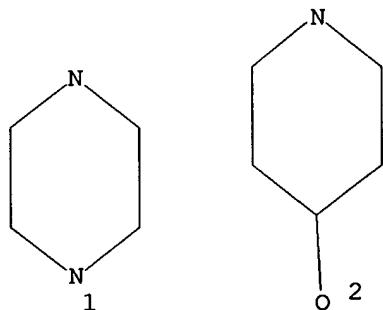
G1 C,O,S,N,X,Cy,[@1],[@2]

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam
SAMPLE SEARCH INITIATED 07:40:48 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   36072 TO ITERATE

   5.5% PROCESSED   2000 ITERATIONS   50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE   **COMPLETE**
                         BATCH   **COMPLETE**
PROJECTED ITERATIONS: 710094 TO   732786
PROJECTED ANSWERS: 50638 TO   56856

L2   50 SEA SSS SAM L1

=> d scan

L2   50 ANSWERS   REGISTRY COPYRIGHT 2005 ACS on STN
IN   Benzenepropanoic acid, 4-[2-[(2,2,6,6-tetramethyl-4-piperidinyl)amino]-4-
     pyrimidinyl]- (9CI)
MF   C22 H30 N4 O2
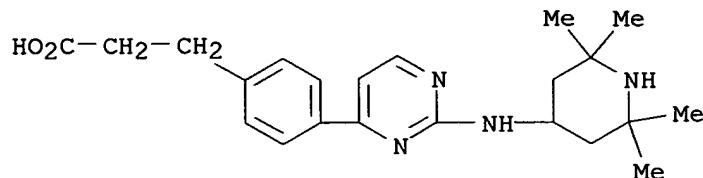
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):49

L2   50 ANSWERS   REGISTRY COPYRIGHT 2005 ACS on STN
IN   1H-Azepin-3-amine, 1-(1-ethylpropyl)-N-[4-(hexahydro-1H-azepin-1-yl)-2-
     pyrimidinyl]hexahydro-, (3S)- (9CI)
MF   C21 H37 N5

Absolute stereochemistry.
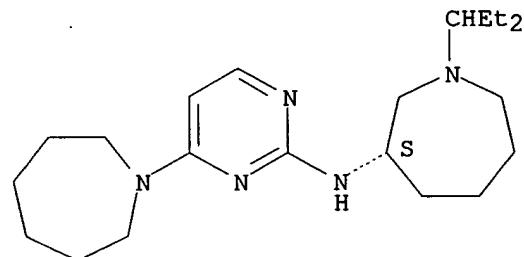
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY COPYRIGHT 2005 ACS on STN
IN   1-Piperidinyloxy, 2,2,6,6-tetramethyl-4-[[[4-methyl-3-[[4-(3-pyridinyl)-2-
     pyrimidinyl]amino]phenyl]amino]carbonyl]- (9CI)
MF   C26 H31 N6 O2
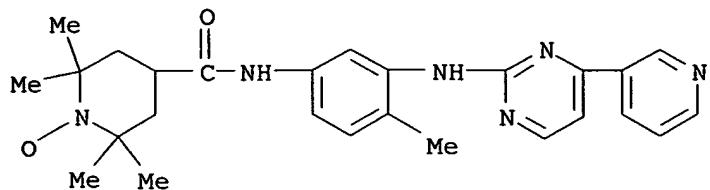
L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   2-Pyrimidinamine, 4-[2-[(2-methoxy-1-methylethyl)amino]-4-pyridinyl]-N-(5-
      methoxy-2-methyl-4-nitrophenyl)- (9CI)
MF   C21 H24 N6 O4
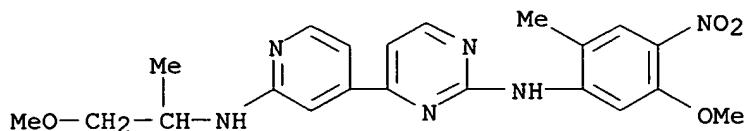
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   2-Pyrimidinamine, N-(1,3-benzodioxol-5-ylmethyl)-4-phenyl- (9CI)
MF   C18 H15 N3 O2
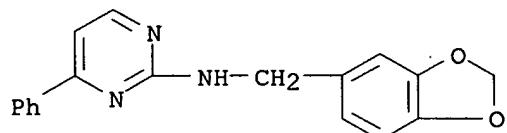
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Carbamic acid, [2-[[3,4-dimethoxy-5-[3-(4-methyl-1-
      piperazinyl)propoxy]phenyl]amino]-4-pyrimidinyl][2-methoxy-4-[[(1-
      methylpropyl)amino]carbonyl]phenyl]-, 2,6-dimethylphenyl ester (9CI)
MF   C41 H53 N7 O7
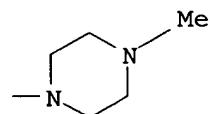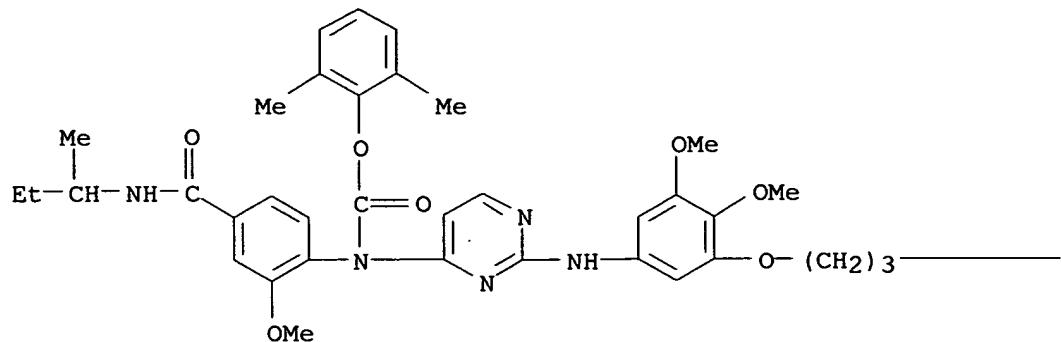
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   2,4-Pyrimidinediamine, N2,N2'-1,6-hexanediylbis[N4-(4-chlorophenyl)-,
      dihydrochloride (9CI)
MF   C26 H28 Cl2 N8 . 2 Cl H
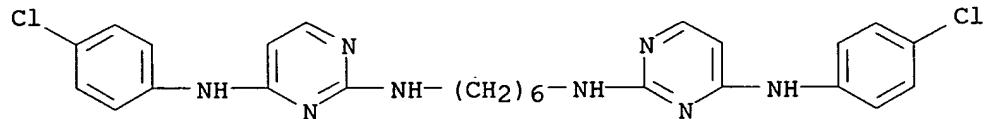
●2 HCl

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Methanesulfonamide, N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-
      pyrimidinyl]phenyl]methyl]-N-ethyl- (9CI)
MF   C22 H25 Cl N4 O3 S
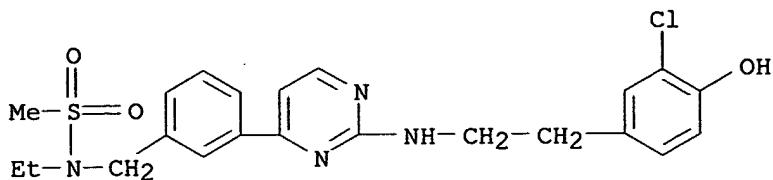
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Cadmium, bis(4-amino-2(1H)-pyrimidinone-κN3)bis(N-benzoylglycinato-
      κO)-, (T-4)- (9CI)
MF   C26 H26 Cd N8 O8
CI   CCS, COM
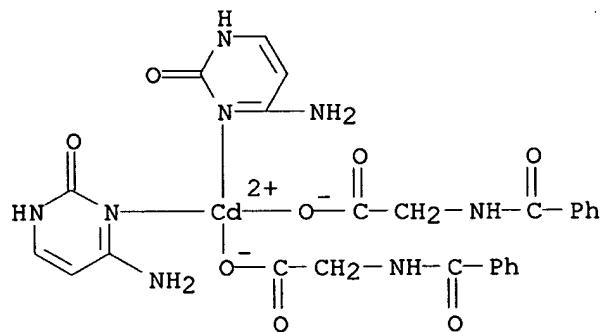
L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   [1,4'-Bipiperidine]-1'-carboxamide, 3-[[4-(hexahydro-1H-azepin-1-yl)-2-
      pyrimidinyl]amino]-N-(2-phenylethyl)- (9CI)
MF   C29 H43 N7 O
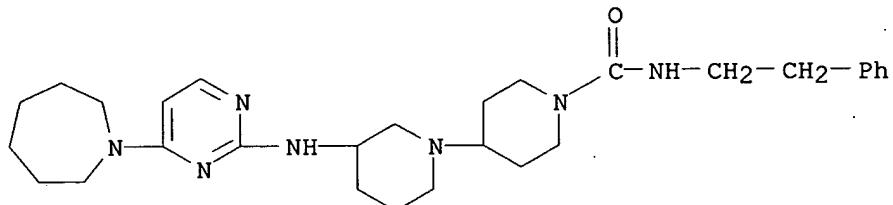
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Piperazine, 1-acetyl-4-[[4-[[[4-[cyano[6-(trifluoromethyl)-2-
      benzothiazolyl]methyl]-2-pyrimidinyl]oxy]methyl]phenyl]methyl]- (9CI)
MF   C28 H25 F3 N6 O2 S
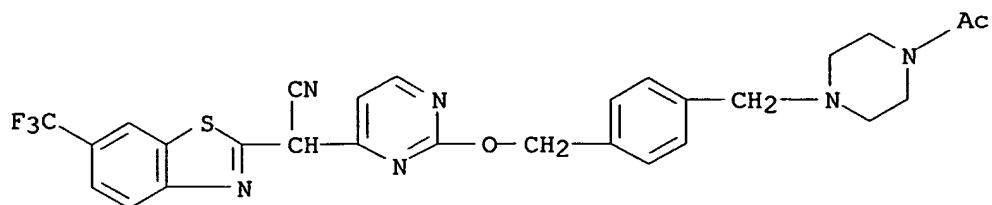
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   3H-Pyrazole-3-thione, 2-[4-[2-[(3-chlorophenyl)amino]-4-pyrimidinyl]-2-
      pyridinyl]-2,4-dihydro-4,5-dimethyl- (9CI)
MF   C20 H17 Cl N6 S
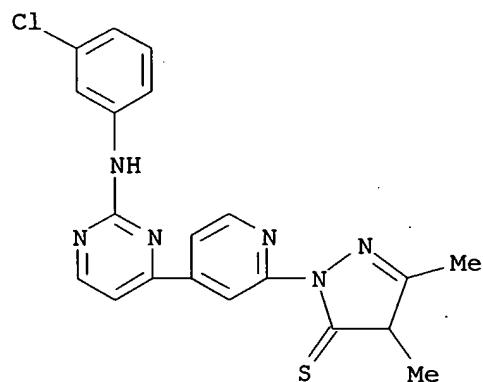
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Pyrimidine, 4-(4-chlorophenyl)-2-(4-methyl-1-piperidinyl)- (9CI)
MF   C16 H18 Cl N3
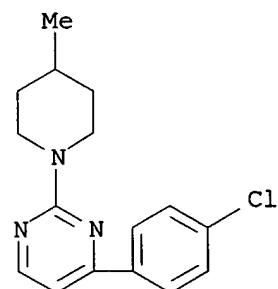
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   1-Azabicyclo[2.2.2]octan-3-amine, N-[4-[6-(4-fluorophenyl)imidazo[2,1-
      b]oxazol-5-yl]-2-pyrimidinyl]- (9CI)
MF   C22 H21 F N6 O
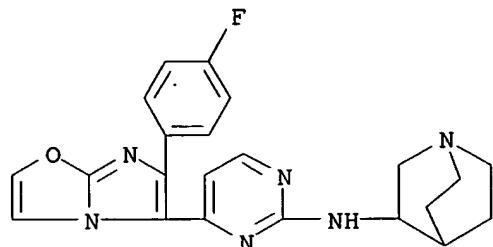
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   4H-Pyrrolo[3,2-c]pyridin-4-one, 2-[2-(2-bromo-4-ethoxy-5-methoxyphenyl)-4-
      pyrimidinyl]-1,5,6,7-tetrahydro- (9CI)
MF   C20 H19 Br N4 O3
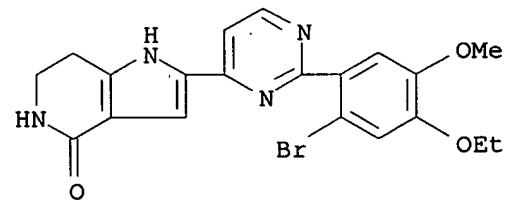
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Pyrimidine, 2-amino-4-(3-aminopropylamino)- (5CI)
MF   C7 H13 N5
CI   COM
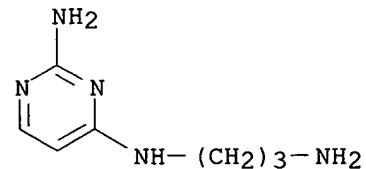
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Benzamide, N-[cis-4-[[4-(dimethylamino)-2-pyrimidinyl]amino]cyclohexyl]-
      3,4,5-trifluoro-, monohydrochloride (9CI)
MF   C19 H22 F3 N5 O . Cl H

Relative stereochemistry.

● HCl
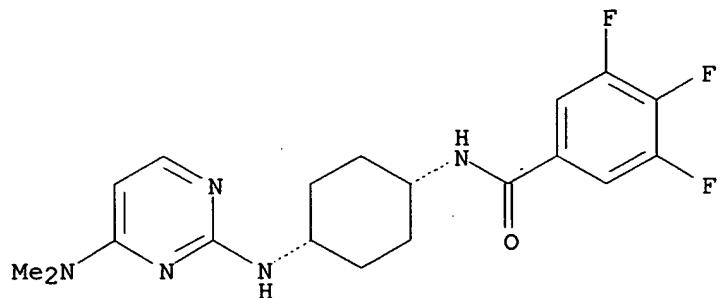
L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   2-Pyrimidinamine, N-(1-cyclobutyl-3-pyrrolidinyl)-4-(hexahydro-1H-azepin-1-
      yl)- (9CI)
MF   C18 H29 N5
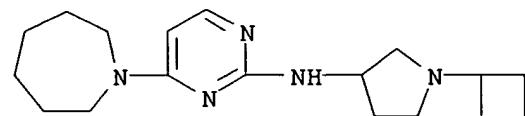
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Piperazine, 1-[5-(methylsulfonyl)-2-(2,2,2-trifluoroethoxy)benzoyl]-4-[4-
      (trifluoromethyl)-2-pyrimidinyl]- (9CI)
MF   C19 H18 F6 N4 O4 S
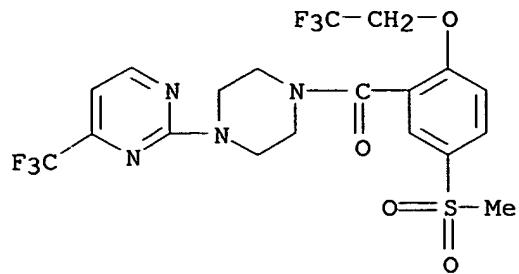
F3C—CH2—O

F3C—[pyrimidine]—N[piperazine]N—C(=O)—[benzene ring with O=S(=O)—Me]

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Spiro[1,3-dioxolane-2,2'(3'H)-[1H,5H]pyrazolo[1,2-a]pyrazol]-5'-one,
      7'-[2-[[(4-aminophenyl)methyl]amino]-4-pyrimidinyl]-6'-(4-fluorophenyl)-
      (9CI)
MF   C25 H23 F N6 O3
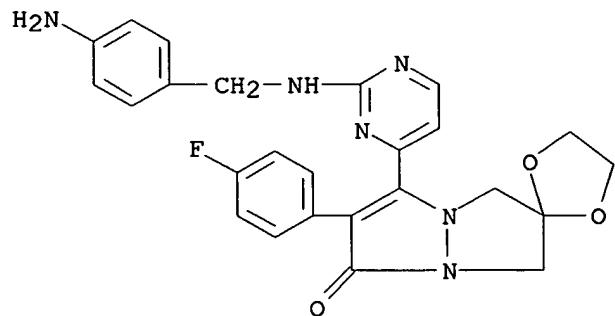
H2N—[phenyl]—CH2—NH—[pyrimidine]—[spiro pyrazolo pyrazolone with 1,3-dioxolane, F-phenyl substituent, O]

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Alanine, N-[[2-[2-(methylamino)-4-pyrimidinyl]-1H-benzimidazol-5-
      yl]carbonyl]-3-(phenyl-2-pyridinylamino)-, methyl ester (9CI)
MF   C28 H26 N8 O3
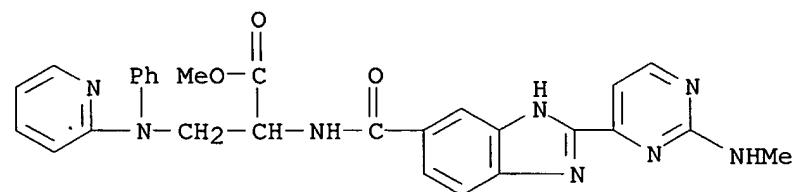
[pyridine]—N(Ph)—CH2—CH(C(=O)OMe)—NH—C(=O)—[benzimidazole]—[pyrimidine]—NHMe

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
      3-[(E)-(1-cyclopropyl-2-oxo-3-pyrrolidinylidene)methyl]-7-[[[(1,4-dihydro-
      4-oxo-2-pyrimidinyl)thio]acetyl]amino]-8-oxo-, (6R,7R)- (9CI)
MF   C21 H21 N5 O6 S2
CI   COM

Absolute stereochemistry.
Double bond geometry as shown.
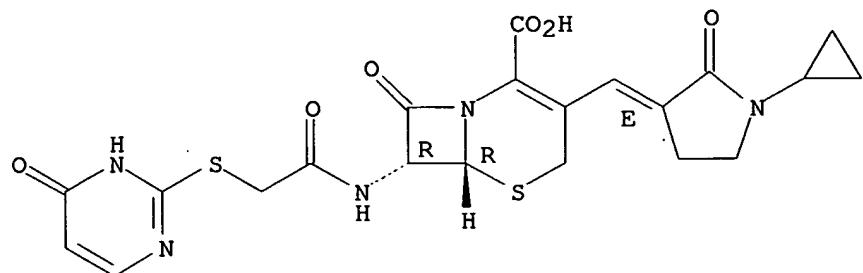
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   2-Pyrimidinamine, N-hexyl-N-methyl-4-[4-(phenylmethyl)-1-piperidinyl]-
      (9CI)
MF   C23 H34 N4
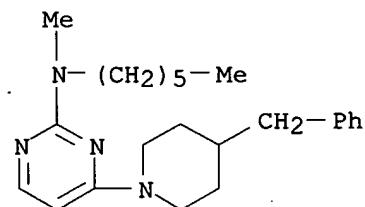
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Glycine, N-[(2,3-dihydro-5-benzofuranyl)carbonyl]-N-[2-[(1-
      methylethyl)amino]-4-pyrimidinyl]-, 1,1-dimethylethyl ester (9CI)
MF   C22 H28 N4 O4
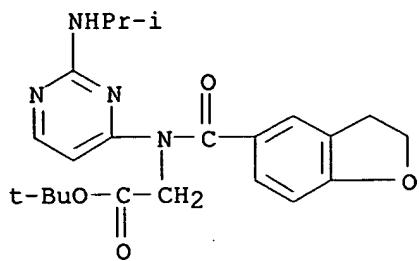
NHPr-i

t-BuO—C—CH2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   2,4-Pyrimidinediamine, N2-[cis-4-[[2-(4-bromophenyl)ethyl]amino]cyclohexyl
      ]-N4,N4-dimethyl- (9CI)
MF   C20 H28 Br N5

Relative stereochemistry.
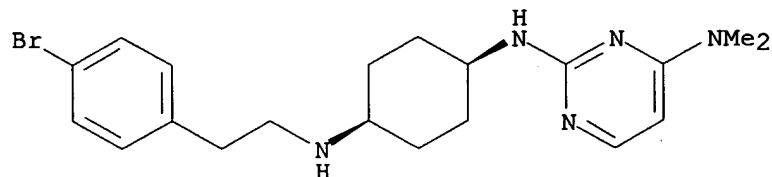
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   4(1H)-Pyrimidinone, 2-[(2-hydroxyphenyl)amino]- (9CI)
MF   C10 H9 N3 O2
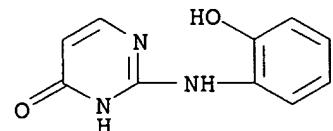
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Carbamic acid, (2-chloro-4-pyrimidinyl)[(2-methoxyphenyl)methyl]-,
      2,6-dimethylphenyl ester (9CI)
MF   C21 H20 Cl N3 O3
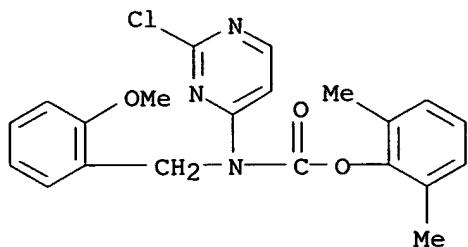
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   1H-Indene-3-acetonitrile, 6-chloro-5-[[2-[(4-cyanophenyl)amino]-4-
      pyrimidinyl]amino]- (9CI)
MF   C22 H15 Cl N6
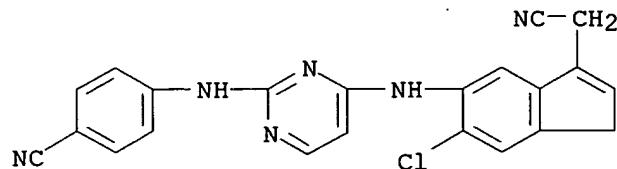
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[(2-ethyl-1-
   piperazinyl)methyl]phenyl]- (9CI)
MF   C25 H29 F2 N5
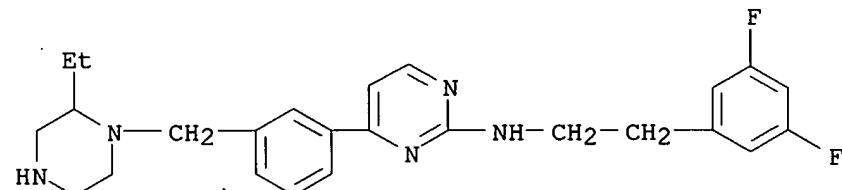
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   2H-Imidazol-2-one, 4-[2-[(2,2-dimethylpropyl)amino]-4-pyrimidinyl]-3-(4-
      fluorophenyl)-1,3-dihydro-1-(tetrahydro-2H-pyran-4-yl)-, monohydrochloride
      (9CI)
MF   C23 H28 F N5 O2 . Cl H

Me3C—CH2—NH

● HCl
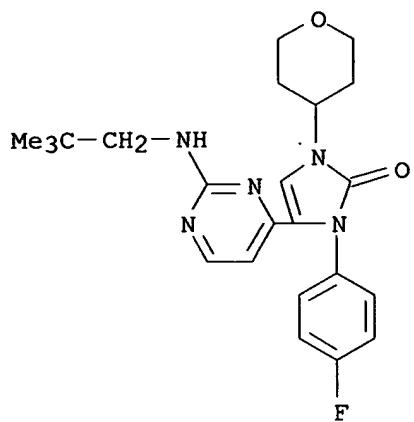
L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Butanoic acid, 4-[[2-[[4-(hexahydro-1H-azepin-1-yl)-2-
      pyrimidinyl]amino]ethyl]methylamino]- (9CI)
MF   C17 H29 N5 O2
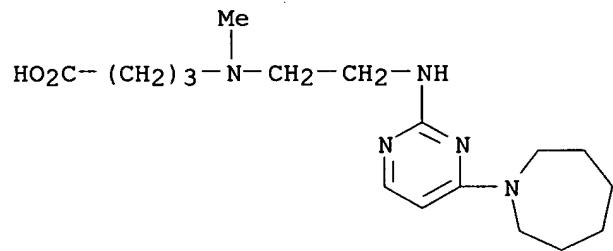
Me
|
HO2C—(CH2)3—N—CH2—CH2—NH

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Benzenesulfonamide, N-cyclopropyl-2-[[2-[(3,4,5-trimethoxyphenyl)amino]-4-
      pyrimidinyl]amino]- (9CI)
MF   C22 H25 N5 O5 S
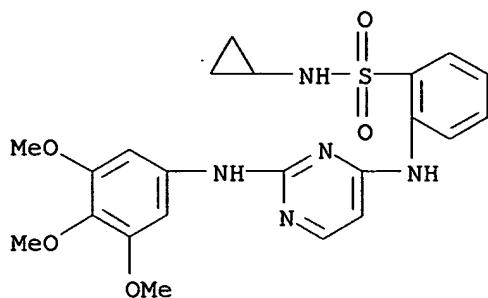
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   1-Piperazinecarboxamide, 4-[4-[(2-amino-4-pyrimidinyl)methoxy]-1,2,5-
      thiadiazol-3-yl]-N-(3,5-diethylphenyl)- (9CI)
MF   C22 H28 N8 O2 S
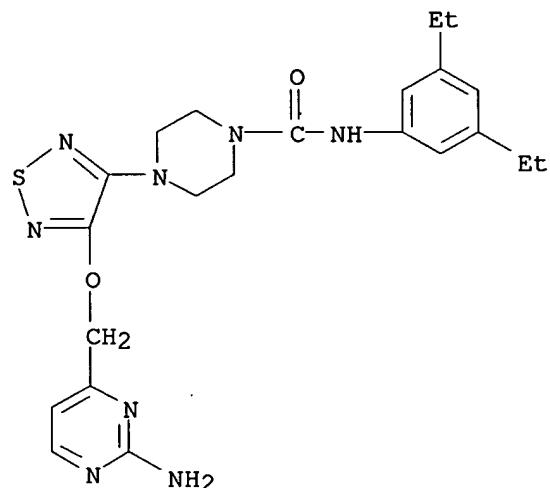
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   2-Piperidinemethanol, 1-[4-(3-pyridinyl)-2-pyrimidinyl]- (9CI)
MF   C15 H18 N4 O
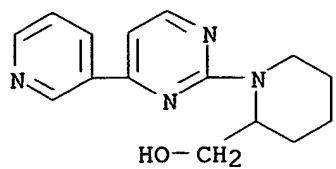
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Carbamic acid, (2,4-dimethoxyphenyl)[2-[[3-fluoro-4-[2-[4-(1-methylethyl)-
      1-piperazinyl]ethoxy]phenyl]amino]-4-pyrimidinyl]-, 2-methyl-1-(1-
      methylethyl)propyl ester (9CI)
MF   C35 H49 F N6 O5
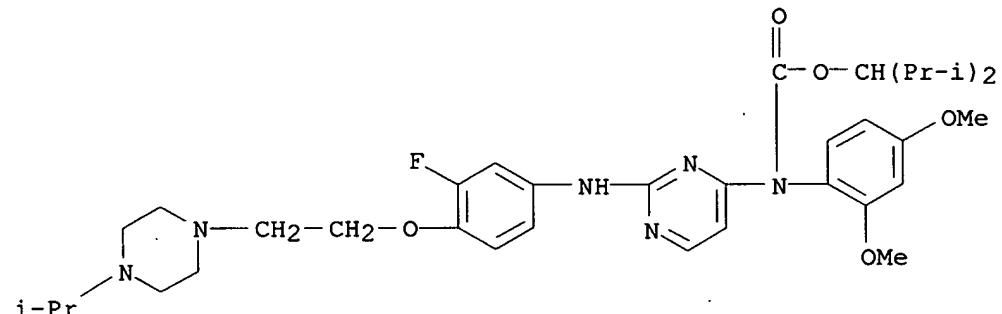

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Benzamide, 4-[(1,1-dioxido-4-oxo-1,2,5-thiadiazolidin-2-yl)methyl]-N-[4-
      methyl-3-[(4-phenyl-2-pyrimidinyl)amino]phenyl]- (9CI)
MF   C27 H24 N6 O4 S
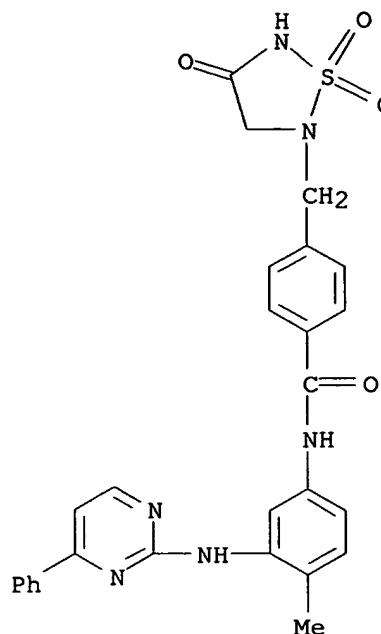
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Benzamide, N-[3-([4,5'-bipyrimidin]-2-ylamino)-4-methylphenyl]-4-[[4-(2-
      hydroxyethyl)-1-piperazinyl]methyl]-3-(trifluoromethyl)- (9CI)
MF   C30 H31 F3 N8 O2
CI   COM

PAGE 1-A
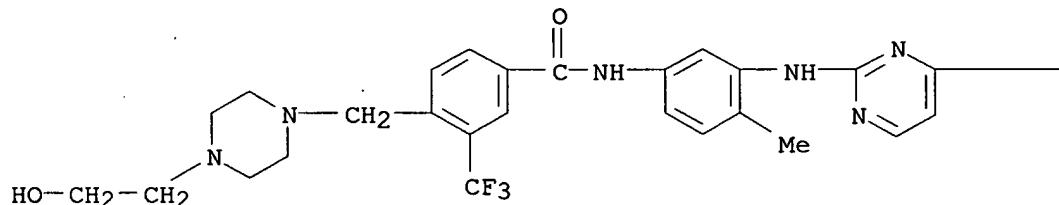
PAGE 1-B
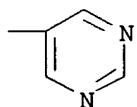
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   2-Pyrimidinamine, N-(3,5-dimethoxyphenyl)-4-[5-(2-methoxyethyl)-4-methyl-2-
      thiazolyl]- (9CI)
MF   C19 H22 N4 O3 S
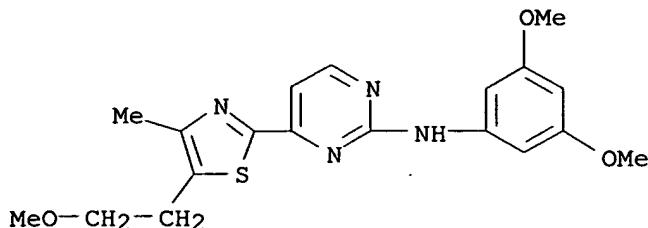
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   [1,4'-Bipiperidin]-3-amine, N-[4-(hexahydro-1H-azepin-1-yl)-2-pyrimidinyl]-
      1'-(4-methoxybenzoyl)- (9CI)
MF   C28 H40 N6 O2
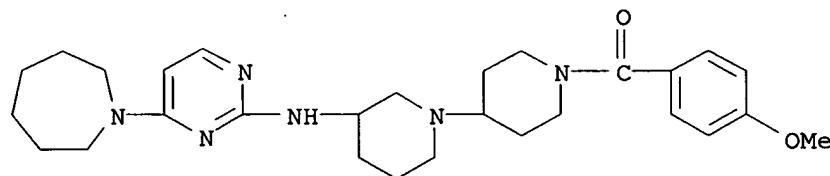
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   6H-Purin-6-one, 2-amino-1,7-dihydro-, compd. with 4-amino-2(1H)-
      pyrimidinone (1:1), radical ion(1+) (9CI)
MF   C5 H5 N5 O . C4 H5 N3 O

      CM   1
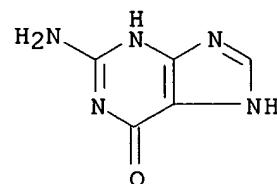
      CM   2
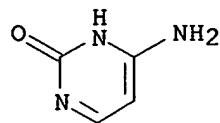
L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   2H-Imidazol-2-one, 1-(cyclopropylmethyl)-3-(4-fluorophenyl)-1,3-dihydro-4-
      [2-[(trans-4-hydroxycyclohexyl)amino]-4-pyrimidinyl]- (9CI)
MF   C23 H26 F N5 O2
CI   COM

Relative stereochemistry.
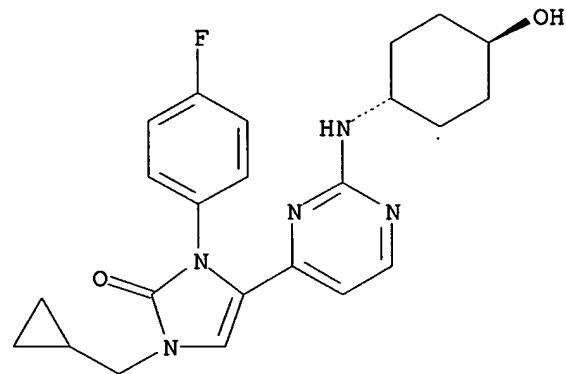
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT


L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   1,3-Benzenedicarboxamide, N'-[(1S)-2-amino-1-[(3,5-difluorophenyl)methyl]-
      3-[(4-ethyl-2-pyrimidinyl)methoxy]propyl]-5-(2-oxazolyl)-N,N-dipropyl-
      (9CI)
MF   C34 H40 F2 N6 O4

Absolute stereochemistry.
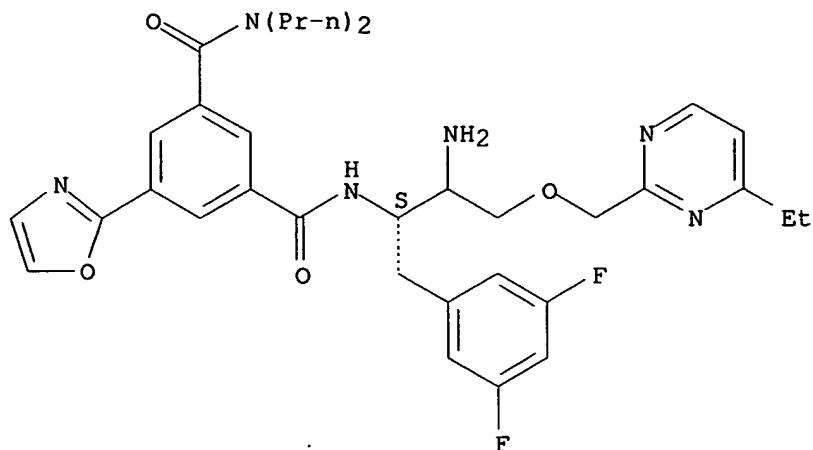
L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   4-Pyrimidineacetonitrile, 2-[[3-(2-oxo-1-pyrrolidinyl)propyl]amino]-
      α-2(1H)-pyridinylidene- (9CI)
MF   C18 H20 N6 O
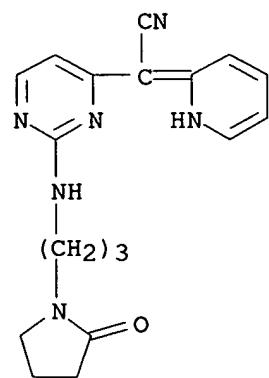
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Ethanedione, phenyl[4-[4-(4,5,6,7-tetrahydro-4-oxo-1H-pyrrolo[3,2-
      c]pyridin-2-yl)-2-pyrimidinyl]phenyl]- (9CI)
MF   C25 H18 N4 O3
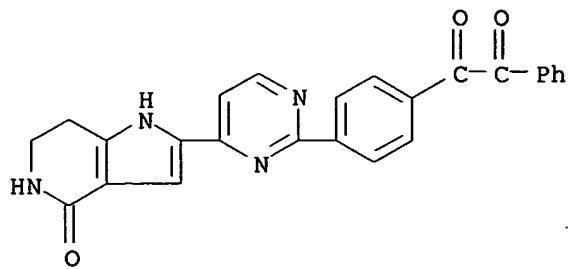
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   2-Pyrimidinamine, 4-(2-methoxyethoxy)- (9CI)
MF   C7 H11 N3 O2
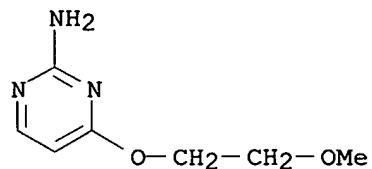
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Urea, N-(4-bromo-2-methylphenyl)-N'-[cis-4-[[4-(dimethylamino)-2-
      pyrimidinyl]amino]cyclohexyl]- (9CI)
MF   C20 H27 Br N6 O

Relative stereochemistry.
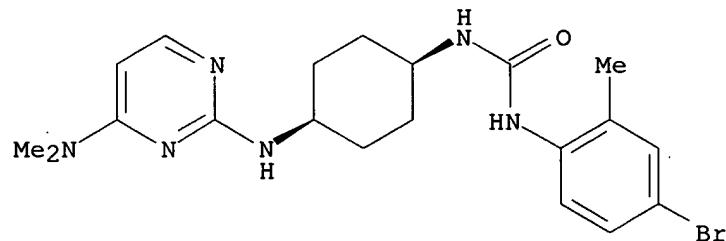
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Benzoic acid, 5-[2-(phenylamino)-4-pyrimidinyl]-2-[[(3R)-tetrahydro-3-
   furanyl]oxy]- (9CI)
MF   C21 H19 N3 O4

Absolute stereochemistry.
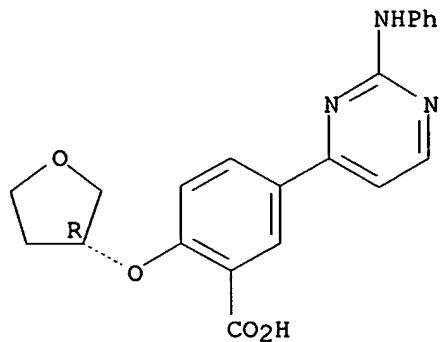
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Benzenesulfonamide, 3-[5-[[3-(2-amino-4-pyrimidinyl)phenyl]amino]-3H-1,2,3-
      triazolo[4,5-d]pyrimidin-3-yl]- (9CI)
MF   C20 H16 N10 O2 S
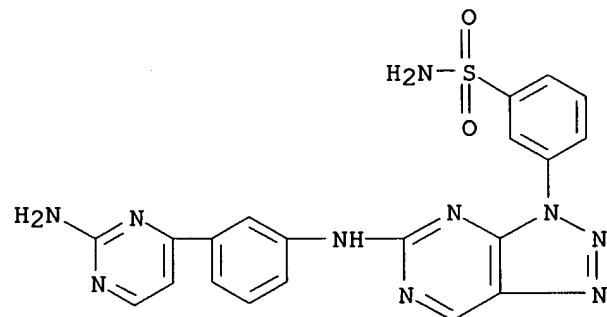
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY   COPYRIGHT 2005 ACS on STN
IN   Benzoic acid, 3-[[4-[2-chloro-4-(trifluoromethyl)-5-thiazolyl]-2-
      pyrimidinyl]amino]-, ethyl ester (9CI)
MF   C17 H12 Cl F3 N4 O2 S
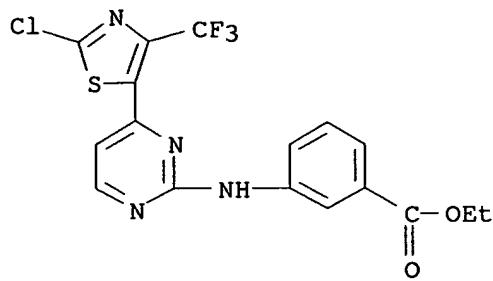
Cl — thiazole ring (N, S), CF3

pyrimidine (N, N) — NH — phenyl — C—OEt, ‖ O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2   50 ANSWERS   REGISTRY COPYRIGHT 2005 ACS on STN
IN   2-Pyrimidinecarbonitrile, 4-[(2,2-dimethylpropyl)[[4-(3-
     hydroxypropyl)phenyl]methyl]amino]- (9CI)
MF   C20 H26 N4 O

NC — pyrimidine (N, N) — N(CH$_2$—CMe$_3$)—CH$_2$ — phenyl — (CH$_2$)$_3$—OH
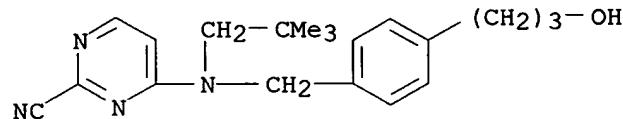
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> log y

| COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.86	1.07

STN INTERNATIONAL LOGOFF AT 07:41:24 ON 01 OCT 2005
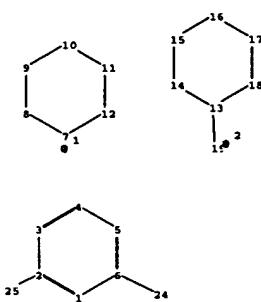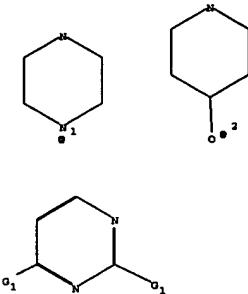
```
chain nodes :
    19   24   25
ring nodes :
    1   2   3   4   5   6   7   8   9   10   11   12   13   14   15   16   17   18
chain bonds :
    2-25   6-24   13-19
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   7-8   7-12   8-9   9-10   10-11   11-12   13-14   13-18   14-15
    15-16   16-17   17-18
exact/norm bonds :
    2-25   6-24   13-19
exact bonds :
    7-8   7-12   8-9   9-10   10-11   11-12   13-14   13-18   14-15   15-16   16-17   17-18
normalized bonds :
    1-2   1-6   2-3   3-4   4-5   5-6
isolated ring systems :
    containing 1 : 7 : 13 :


G1:[*1],[*2]

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom   10:Atom   11:Atom
    12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   18:Atom   19:CLASS   24:CLASS   25:CLASS
```